Theory, Modeling, and Simulation

Opportunity

The emergence of new behaviors and processes in nanomaterials, nanostructures, nanodevices, and nanosystems creates an urgent need for theory, modeling, large-scale computer simulation, and new design tools in order to understand, control, and accelerate development.

Priorities

Research on mathematical methods to model and simulate physical, chemical, and biological systems at the nanoscale will include techniques such as quantum mechanics and quantum chemistry, multi-particle simulation, molecular simulation, continuum-based models, stochastic methods, and nanomechanics. Approaches that integrate more than one such technique will play an important role in this effort.

Modeling and simulation of the time variation of processes in nanostructures is also an urgent need. Current research is limited to modeling only a relatively small number of time increments of process variation and dynamics of complex structures, such as shown in Figure 6. Improved computational methods and tools will enable more realistic time scales of process variation to be modeled.

Research Example: Modeling and Simulation of Biological Ion Channels to Cure Illnesses (supported by NSF and DOD)

Researchers from the Network for Computational Nanotechnology at the University of Illinois at Urbana-Champaign and Stanford University, in collaboration with Rush Medical Center, have simulated transport through nanoscale biological ion channels (Figure 6). Ion channels regulate the transport of ions in and out of cells, which is essential to proper cell function. In turn, understanding cellular processes is critical to understanding and treating diseases at the cellular level.

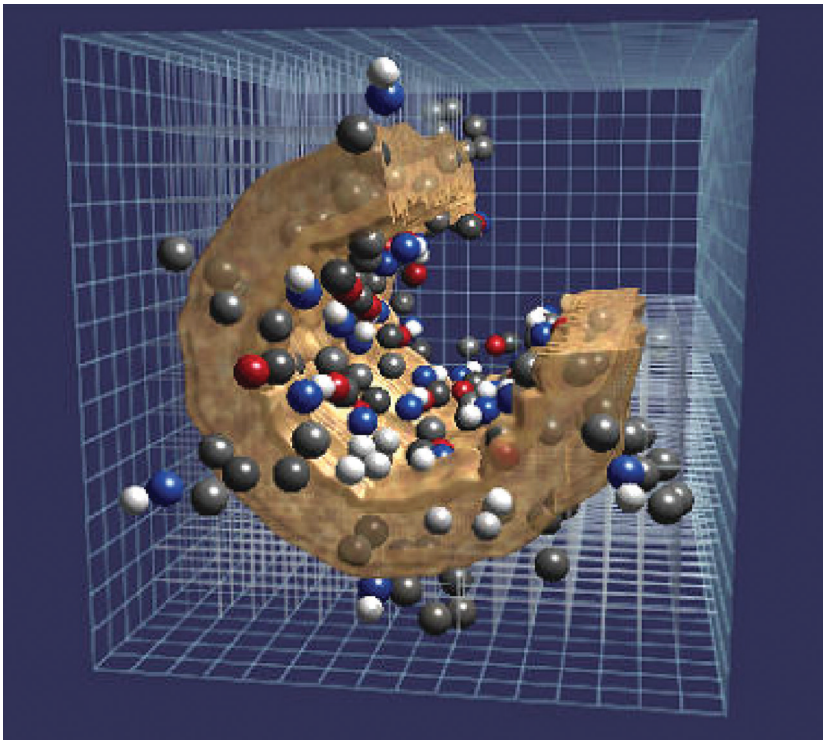

Figure 6. Computer simulation of biological ion-channel pore formed by the antibiotic gramicidin. Formation of ion channels through bacteria cell membranes is one mechanism by which antibiotics kill bacteria. The simulated pore is approximately 3 nanometers long and 0.5 nanometers in diameter. The different colored spheres represent specific atoms in the proteins constituting the wall of the ion channel (courtesy K. Hess and U. Ravaioli, University of Illinois).